IMPLEMENTATION OF THE COMPARATIVE MODELING EVALUATION

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We provide a description of the criteria used in the evaluation program. The measures applied include RMS deviations in atomic positions and dihedral angles as well as deviations in error estimates. Several exclusions are employed to filter out the influence of possible experimental uncertainties. These include thermal motion, disorder, intermolecular contacts in the crystal, and atomic assignment deemed unreliable crystallographically. A number of subsets select for regions of structure particularly difficult to predict. These subsets allow to focus on sidechains which are rotamerically different in the parent structure, structure segments shifted relative to parent, favorable alternative parent selections, and loops. The last group of subsets specifies surface and core regions, as well as regions of structure in contact with ligand(s).